

Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -20.7 °C

Global applicability domain: Inside

Local applicability domain index: 6.83e-01

Confidence level: 4.81e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Hexachloro-1,3-butadiene</div> <div>Measured: -21.0</div> <div>Predicted: -20.7</div>	<div>Image not found</div> <div>Hexachlorocyclopentadiene</div> <div>Measured: -9.00</div> <div>Predicted: 2.05</div>	<div>Image not found</div> <div>Hexachloropropene</div> <div>Measured: -72.9</div> <div>Predicted: -34.7</div>
<div>Image not found</div> <div>Octachlorocyclopentene</div> <div>Measured: 40.0</div> <div>Predicted: 22.2</div>	<div>Image not found</div> <div>Tetrachloroethylene</div> <div>Measured: -22.3</div> <div>Predicted: -13.3</div>	